

10/552,459

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NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 MAY 01 New CAS web site launched
NEWS 3 MAY 08 CA/CAplus Indian patent publication number format defined
NEWS 4 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and
display fields
NEWS 5 MAY 21 BIOSIS reloaded and enhanced with archival data
NEWS 6 MAY 21 TOXCENTER enhanced with BIOSIS reload
NEWS 7 MAY 21 CA/CAplus enhanced with additional kind codes for German
patents
NEWS 8 MAY 22 CA/CAplus enhanced with IPC reclassification in Japanese
patents
NEWS 9 JUN 27 CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 10 JUN 29 STN Viewer now available
NEWS 11 JUN 29 STN Express, Version 8.2, now available
NEWS 12 JUL 02 LEMBASE coverage updated
NEWS 13 JUL 02 LMEDLINE coverage updated
NEWS 14 JUL 02 SCISEARCH enhanced with complete author names
NEWS 15 JUL 02 CHEMCATS accession numbers revised
NEWS 16 JUL 02 CA/CAplus enhanced with utility model patents from China
NEWS 17 JUL 16 CAplus enhanced with French and German abstracts
NEWS 18 JUL 18 CA/CAplus patent coverage enhanced
NEWS 19 JUL 26 USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 20 JUL 30 USGENE now available on STN
NEWS 21 AUG 06 CAS REGISTRY enhanced with new experimental property tags
NEWS 22 AUG 06 BEILSTEIN updated with new compounds
NEWS 23 AUG 06 FSTA enhanced with new thesaurus edition
NEWS 24 AUG 13 CA/CAplus enhanced with additional kind codes for granted
patents
NEWS 25 AUG 20 CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 26 AUG 27 Full-text patent databases enhanced with predefined
patent family display formats from INPADOCDB
NEWS 27 AUG 27 USPATOLD now available on STN
NEWS 28 AUG 28 CAS REGISTRY enhanced with additional experimental
spectral property data

10/552, 459

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

| | |
|------------|---|
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STRUCTURE FILE UPDATES: 31 AUG 2007 HIGHEST RN 945948-91-4
DICTIONARY FILE UPDATES: 31 AUG 2007 HIGHEST RN 945948-91-4

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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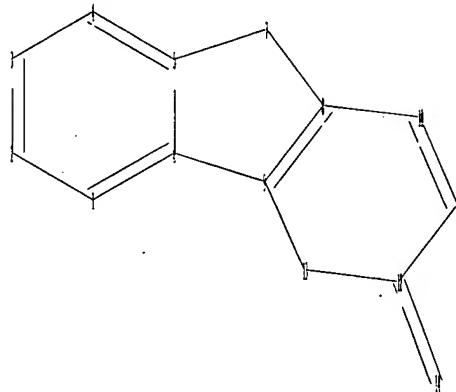
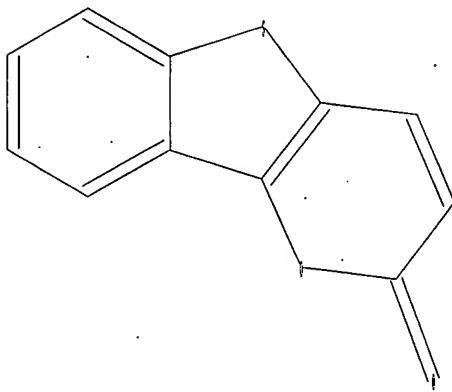
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<http://www.cas.org/support/stn/gen/stndoc/properties.html>

=>

10/552,459

Uploading C:\Program Files\Stnexp\Queries\10552459.str



chain nodes :

14

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

12-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 8-10 9-13 10-11 11-12

12-13

exact/norm bonds :

12-14

exact bonds :

5-7 6-9 7-8 8-9 8-10 9-13 10-11 11-12 12-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:CLASS

L1 STRUCTURE UPLOADED

=> s 11

SAMPLE SEARCH INITIATED 17:47:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS
SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

10/552, 459

PROJECTED ITERATIONS: 1 TO 80
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s 11 ful
FULL SEARCH INITIATED 17:48:02 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 56 TO ITERATE

100.0% PROCESSED 56 ITERATIONS 52 ANSWERS
SEARCH TIME: 00.00.01

L3 52 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION
172.10 172.31

FILE 'CAPLUS' ENTERED AT 17:48:12 ON 02 SEP 2007
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FILE LAST UPDATED: 31 Aug 2007 (20070831/ED)

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<http://www.cas.org/infopolicy.html>

=> s 13
L4 16 L3

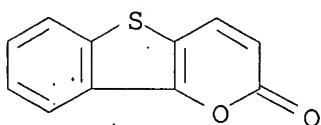
=> d 14 ibib hitstr abs

L4 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:902391 CAPLUS
DOCUMENT NUMBER: 141:370267
TITLE: Fragrance compositions comprising
benzo[4,5]thieno[3,2-

INVENTOR(S): b]pyran-2-one
 Turin, Luca
 PATENT ASSIGNEE(S): Flexitral, Inc., USA
 SOURCE: PCT Int. Appl., 28 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|------------------|------------|
| WO 2004092182 | A1 | 20041028 | WO 2004-US10829 | 20040408 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
TD, TG | | | | |
| AU 2004230923 | A1 | 20041028 | AU 2004-230923 | 20040408 |
| CA 2521834 | A1 | 20041028 | CA 2004-2521834 | 20040408 |
| EP 1622915 | A1 | 20060208 | EP 2004-759279 | 20040408 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK | | | | |
| GB 2418915 | A | 20060412 | GB 2005-22412 | 20040408 |
| CN 1784411 | A | 20060607 | CN 2004-80012014 | 20040408 |
| JP 2006526623 | T | 20061124 | JP 2006-509812 | 20040408 |
| US 2006292097 | A1 | 20061228 | US 2006-552459✓ | 20060804 |
| PRIORITY APPLN. INFO.: | | | US 2003-461090P | P 20030408 |
| | | | WO 2004-US10829 | W 20040408 |

IT 5732-22-9P, Tonkene
 RL: COS (Cosmetic use); FFD (Food or feed use); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)
 (preparation of aromachems. for fragrances and flavorings)
 RN 5732-22-9 CAPLUS
 CN 2H-[1]Benzothieno[3,2-b]pyran-2-one (8CI, 9CI) (CA INDEX NAME)



10/552,459

AB The present invention relates to perfumes and other fragrant articles based on aromachems. which overcome the stability limitations and/or allergenic nature of the native compds. Particularly, compns. comprising at least 30% of benzo[4,5]thieno[3,2-b]pyran-2-one employed as aroma chemical for fragrances and flavorings are described. For example, benzo[4,5]thieno[3,2-b]pyran-2-one was synthesized by reacting 2-mercaptopbenzoic acid with trans-glutaconic acid in the presence of a catalytic amount of sulfuric acid.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 14 ibib hitstr abs 2-16

L4 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:351145 CAPLUS

DOCUMENT NUMBER: 129:31781

TITLE: Biodegradation of dibenzothiophene by a nodulating isolate of Rhizobium meliloti

AUTHOR(S): Frassinetti, Stefania; Setti, Leonardo; Corti, Andrea;

Farrinelli, Paolo; Montevercchi, Piercarlo; Vallini, Giovanni

CORPORATE SOURCE: National Research Council (CNR), Soil Microbiology Center, Pisa, 56124, Italy

SOURCE: Canadian Journal of Microbiology (1998), 44(3), 289-297

CODEN: CJMIAZ; ISSN: 0008-4166

PUBLISHER: National Research Council of Canada

DOCUMENT TYPE: Journal

LANGUAGE: English

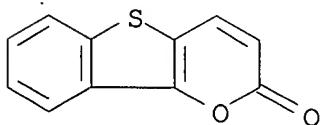
IT 5732-22-9, 2H-[1]Benzothieno[3,2-b]pyran-2-one

RL: BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); REM (Removal or disposal); BIOL (Biological study);

FORM (Formation, nonpreparative); PROC (Process)
(formation of; in biodegrdn. of dibenzothiophene by a nodulating isolate of Rhizobium meliloti).

RN 5732-22-9 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one (8CI, 9CI) (CA INDEX NAME)

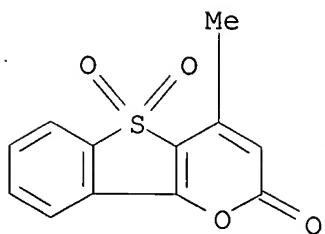


10/552,459

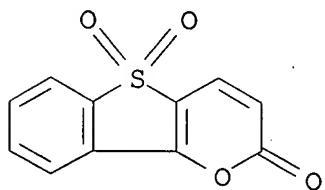
AB Rhizobium meliloti strain Orange 1 was isolated from aerobic sediments of a drainage ditch receiving oil refinery leakage. This bacterium has been shown to be capable of growing on dibenzothiophene as the sole carbon and energy source. This strain can also efficaciously nodulate alfalfa plants. In cultures with dibenzothiophene, strain Orange 1 produces six degradation intermediates. By means of analyses with UV-visible spectrometry and gas chromatog.-mass spectrometry, as well as NMR spectroscopy, three of these products were identified as 3-hydroxy-2-formyl-benzothiophene (product A), benzothienopyran-2-one (product B'), and dibenzothiophene-5-oxide (product D). This suggests that R. meliloti strain Orange 1 metabolizes dibenzothiophene via oxidative cleavage of the aromatic ring with a mechanism analogous to that described for naphthalene degradation
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:154182 CAPLUS
DOCUMENT NUMBER: 110:154182
TITLE: Some reactions of
2H-[1]benzothieno[3,2-b]pyran-2-ones
and related compounds
AUTHOR(S): Buggle, Katherine; Ghogain, Una Ni; MacManus, Patrick
CORPORATE SOURCE: Dep. Chem., Univ. Coll., Dublin, Ire.
SOURCE: Monatshefte fuer Chemie (1988), 119(8-9), 945-51
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:154182
IT 119872-67-2P 119872-68-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(preparation and thiation of)
RN 119872-67-2 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-methyl-, 5,5-dioxide (9CI) (CA INDEX NAME)

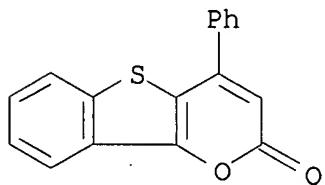
10/552, 459



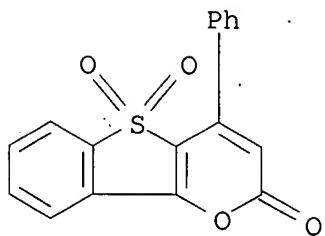
RN 119872-68-3 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 5,5-dioxide (9CI) (CA INDEX NAME)



IT 87894-69-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with acetylenedicarboxylate)
RN 87894-69-7 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-phenyl- (9CI) (CA INDEX NAME)



IT 87894-70-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(thiation or reaction with methylamine)
RN 87894-70-0 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-phenyl-, 5,5-dioxide (9CI) (CA INDEX NAME)

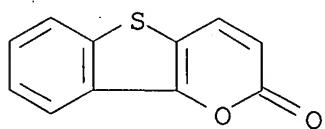


IT 5732-22-9, 2H-[1]Benzothieno[3,2-b]pyran-2-one 119872-66-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(S-oxidation and thiation of)

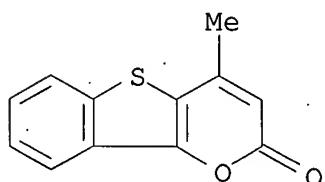
RN 5732-22-9 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one (8CI, 9CI) (CA INDEX NAME)

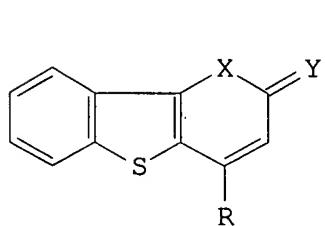


RN 119872-66-1 CAPLUS

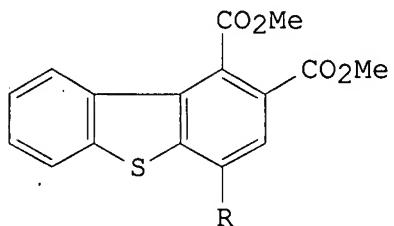
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-methyl- (9CI) (CA INDEX NAME)



GI



I



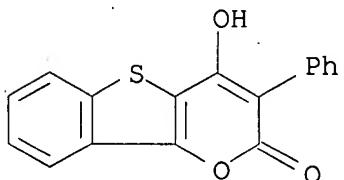
II

AB The conversion of 2H-[1]benzothieno[3,2-b]pyran-2-ones I (X = Y = O, R = Ph; Me, H) into mono- and dithio derivs. and the preparation of some dibenzothiophenes (II) sulfines I (X = S, Y = SO) and pyridones I (X =

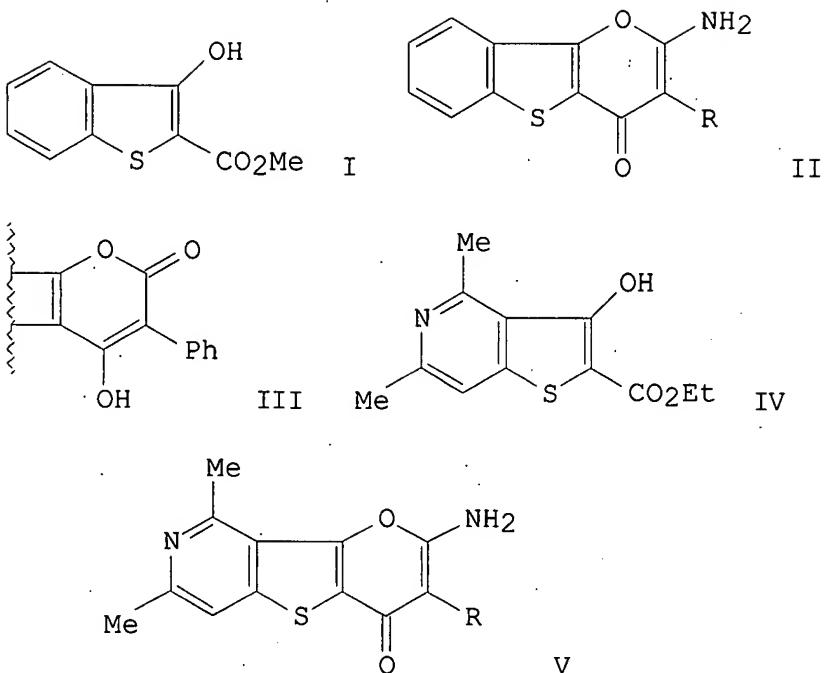
10/552, 459

NMe, Y = O) are described.

L4 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:120920 CAPLUS
DOCUMENT NUMBER: 100:120920
TITLE: Annelation of the 2-aminopyran-4-one ring to
condensed thiophenes
AUTHOR(S): Volovenko, Yu. M.; Litenko, V. A.; Khrapak, T. V.;
Babichev, F. S.
CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, 252017, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii. (1983),
(11), 1476-8
DOCUMENT TYPE: CODEN: KGSSAQ; ISSN: 0453-8234
LANGUAGE: Journal
Russian
OTHER SOURCE(S): CASREACT 100:120920
IT 89155-19-1P RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 89155-19-1 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-phenyl- (9CI) (CA
INDEX NAME)



GI



AB Cyclocondensation of benzothiophenecarboxylate I with RCH₂CN [R = Ph, 2-ClC₆H₄, 2,3,4-(MeO)C₆H₂] catalyzed by Me₂CHONa gave 55-70% II which (R = Ph) was acetylated to give the N-acetyl derivative and hydrolyzed to give 70% III. Similar treatment of thienopyridinecarboxylate IV by RCH₂CN [R = Ph, 2-ClC₆H₄, 3,4-(MeO)C₆H₃] gave 83-90% V.

L4 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1983:612429 CAPLUS

DOCUMENT NUMBER: 99:212429

TITLE: Thiopyrano[1]benzothiophenes. Synthesis of
1-phenyl-3H-thiopyrano[3,4-b][1]benzothiophene
thione 9,9-dioxide and related compounds
AUTHOR(S): Bugle, Katherine; Ghogain, Una Ni; Nangle,

AUTHOR(S): Buggle, Katherine; Ghogain, Una Ni; Nangle,
Michael;

CORPORATE SOURCE: Nachmanus, Patrick
Dep. Chem. Univ.

CORPORATE SOURCE: Dep. Chem., Univ. Coll., Dublin, Ire.
SOURCE: Journal of the Chemical Society, Park

SOURCE: Journal of the Chemical Society, Perkin Transactions

TRANSACTIONS

1: Organic and Bio-Organic Chemistry (1972-1999)
(1983), (7), 1427-9

CODEN: JCPRB4; ISSN: 0300-922X

Journal

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 99:212429

10/552,459

IT 87894-69-7P

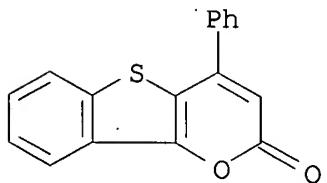
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT

(Reactant or reagent)

(preparation and oxidation of)

RN 87894-69-7 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-phenyl- (9CI) (CA INDEX NAME)



IT 87894-70-0P

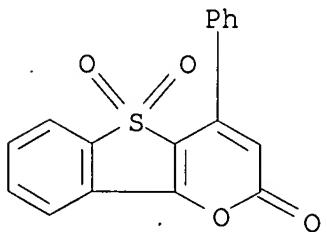
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT

(Reactant or reagent)

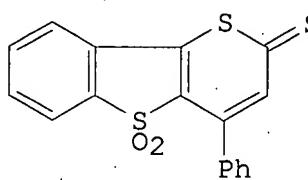
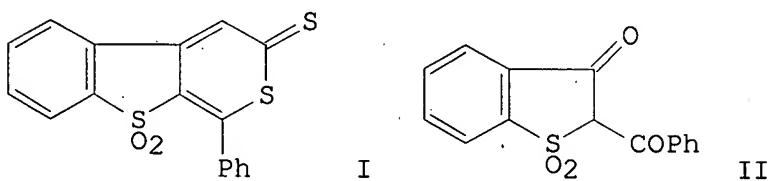
(preparation and sulfuration of)

RN 87894-70-0 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-phenyl-, 5,5-dioxide (9CI) (CA INDEX NAME)



GI



AB The title compound (I) was prepared in 45% yield by the cyclocondensation of benzothiophenone II with P4S10 in refluxing MeCN containing NaHCO3 for 1 h.

The isomeric compound III was prepared by the cyclocondensation of 2-HSC6H4CO2H with HO2CCH2CPh:CHCO2H followed by oxidation and disulfuration.

Several analogs of I and III were also prepared

L4 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1983:53665 CAPLUS

DOCUMENT NUMBER: 98:53665

TITLE: Ring-expansion of some sulfur-containing heterocyclic

AUTHOR(S): compounds with dimethyl acetylenedicarboxylate
Lamm, Bo; Aurell, Carl Johan

CORPORATE SOURCE: Dep. Org. Chem., Chalmers Univ. Technol.,
Goteborg,

SOURCE: S-412 96, Swed.

Acta Chemica Scandinavica, Series B: Organic
Chemistry and Biochemistry (1982), B36(7), 435-42
CODEN: ACBOCV; ISSN: 0302-4369

DOCUMENT TYPE: Journal

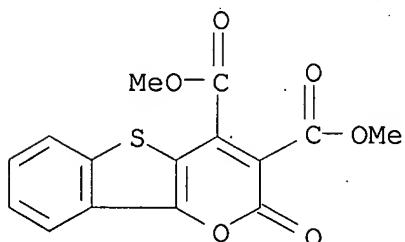
LANGUAGE: English

IT 84261-39-2P

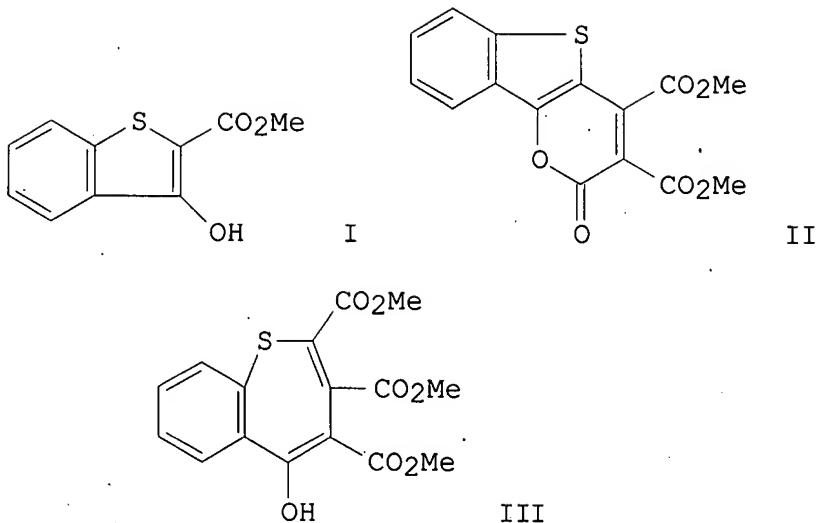
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 84261-39-2 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-3,4-dicarboxylic acid, 2-oxo-, dimethyl ester (9CI) (CA INDEX NAME)

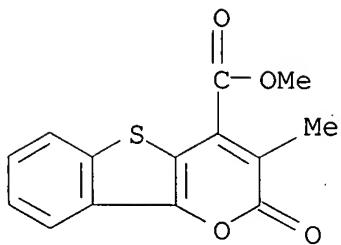


GI

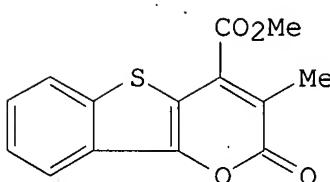
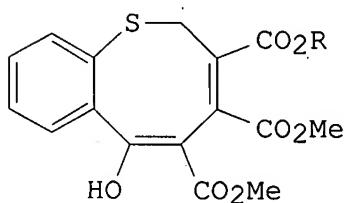


AB Benzo[b]thiepin, benzo[b]thiocin, and benzo[b]thionin derivs. were prepared.

through [2+2] cycloaddn. of di-Me acetylenedicarboxylate to enamines, β -keto-ester anions and one β -diketone anion. In the addition to I a fluorescent by-product was identified as an α -pyrone-derivative (II), besides the main product III.



GI



I

II

AB Thermolysis of the title compound or its Et analog (I, R = Me, Et) gave the benzothienopyranone II. The structure of II was confirmed by independent synthesis from 3-hydroxybenzo[b]thiophene and MeO₂CCHMeCOCO₂Me.

L4 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1978:44882 CAPLUS

DOCUMENT NUMBER: 88:44882

TITLE: Antitumor activity of heterocyclic and ketenethioacetal derivatives

AUTHOR(S): Kobayashi, Goro; Matsuda, Yoshiro; Tominaga, Yoshinori; Ohkuma, Mihoko; Shinoda, Hirotaka; Kohno,

CORPORATE SOURCE: Morihiro; Mizuno, Den'ichi
Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, Japan
SOURCE: Yakugaku Zasshi (1977), 97(9), 1039-45DOCUMENT TYPE: CODEN: YKKZAJ; ISSN: 0031-6903
Journal

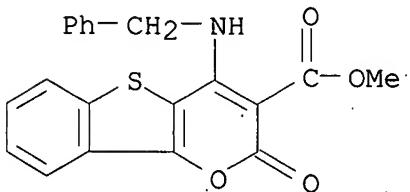
LANGUAGE: Japanese

IT 57840-16-1P

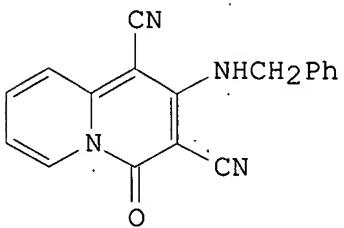
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);BIOL (Biological study); PREP (Preparation); USES (Uses)
(préparation and antitumor activity of)

RN 57840-16-1 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-3-carboxylic acid, 2-oxo-4-[(phenylmethyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



GI



I

AB Eighty-seven compds. of maleimide, five- or six-ring heterocyclic 4H-quinolizines, and ethylene derivs. were prepared and their antitumor activity was examined using a solid type of Ehrlich carcinoma. 1,3-Dicyano-2-benzylamine-4H-quinolizin-4-one (I) [65125-90-8] had some antitumor effect, but no other synthesized compds. were effective.

L4 ANSWER 9 OF 16 CAPLUS, COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:17052 CAPLUS

DOCUMENT NUMBER: 84:17052

TITLE: Heterocyclic ketenethioacetal derivatives. VI. Synthesis and reaction of 2-

bis(methylthio)methylenebenzothiophen-3(2H)-one

Tominaga, Yoshinori; Morita, Yuko; Matsuda, Yoshiro;

Kobayashi, Goro

CORPORATE SOURCE: Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1975), 23(10), 2390-6

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 84:17052

IT 57840-11-6P 57840-12-7P 57840-16-1P

57840-17-2P

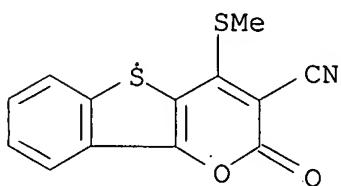
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

10/552,459

RN 57840-11-6 CAPLUS

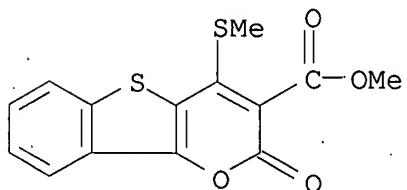
CN 2H-[1]Benzothieno[3,2-b]pyran-3-carbonitrile, 4-(methylthio)-2-oxo-
(9CI)

(CA INDEX NAME)



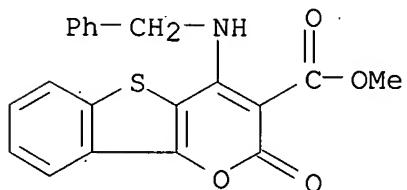
RN 57840-12-7 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-3-carboxylic acid, 4-(methylthio)-2-oxo-,
methyl ester (9CI) (CA INDEX NAME)



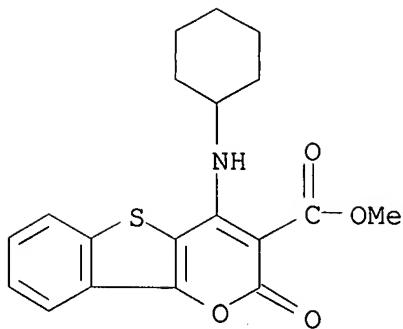
RN 57840-16-1 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-3-carboxylic acid, 2-oxo-4-
[(phenylmethyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



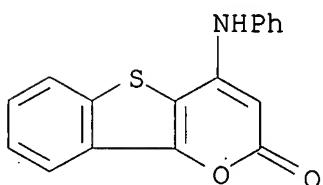
RN 57840-17-2 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-3-carboxylic acid,
4-(cyclohexylamino)-2-oxo-
, methyl ester (9CI) (CA INDEX NAME)



AB 2-Bis (methylthio)methylenebenzothiophen-3(2H)-one, prepared by treatment of benzothiophen-3(2H)-one with CS, in Me₂SO containing NaOH, reacted with nucleophilic reagents such as amines or active methylenes to give the corresponding replacement products of one or two methylthio groups in good yields.

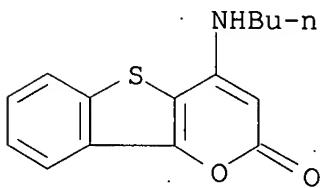
L4 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1975:479110 CAPLUS
 DOCUMENT NUMBER: 83:79110
 TITLE: Action of amines on 4-hydroxy-2-oxo-2H-pyrano[3,2-b]thianaphthalenes
 AUTHOR(S): Ali, Mohamed I.; Samy, Salah M.
 CORPORATE SOURCE: Fac. Sci., Cairo Univ., Giza, Egypt
 SOURCE: Egyptian Journal of Chemistry (1974), Volume Date 1973, (Spec. Issue), 169-77
 CODEN: EGJCA3; ISSN: 0449-2285
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 IT 2035-56-5P 53324-54-2P 53324-55-3P
 53324-56-4P 53324-58-6P 53324-59-7P
 53324-60-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 2035-56-5 CAPLUS
 CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-(phenylamino)- (9CI) (CA INDEX NAME)



10/552, 459

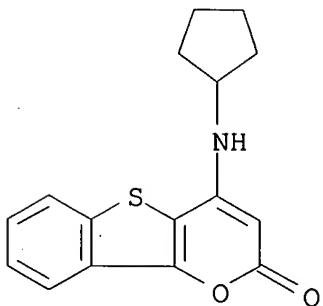
RN 53324-54-2 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-(butylamino)- (9CI) (CA INDEX NAME)



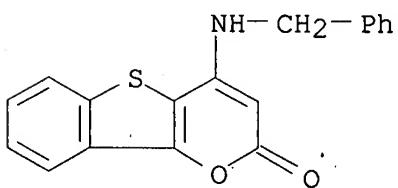
RN 53324-55-3 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-(cyclopentylamino)- (9CI) (CA INDEX NAME)



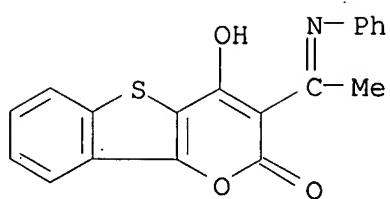
RN 53324-56-4 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-[(phenylmethyl)amino]- (9CI)
(CA INDEX NAME)



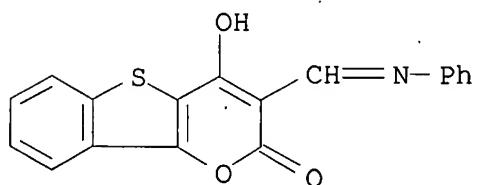
RN 53324-58-6 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one,
4-hydroxy-3-[1-(phenylimino)ethyl]-
(9CI) (CA INDEX NAME)



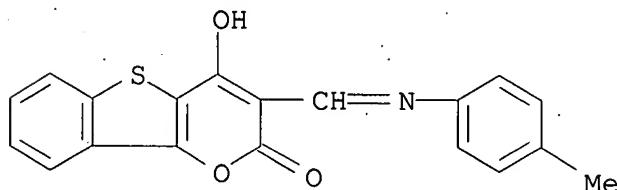
RN 53324-59-7 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-[(phenylimino)methyl]- (9CI) (CA INDEX NAME)



RN 53324-60-0 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-[(4-methylphenyl)imino]methyl- (9CI) (CA INDEX NAME)



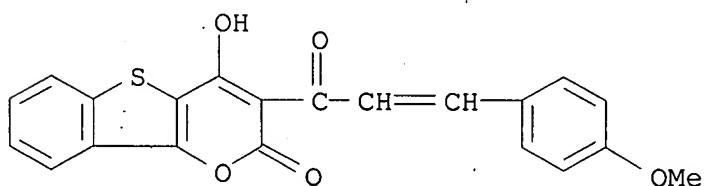
IT 2034-93-7 2035-18-9 6906-77-0

56342-51-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with amines)

RN 2034-93-7 CAPLUS

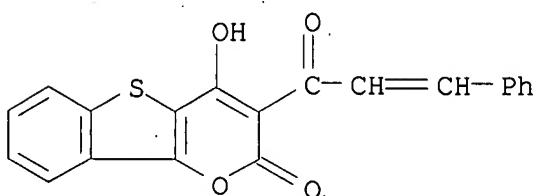
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one,
4-hydroxy-3-[(4-methoxyphenyl)-1-
oxo-2-propenyl]- (9CI) (CA INDEX NAME)



10/552,459

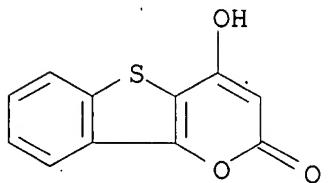
RN 2035-18-9 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(1-oxo-3-phenyl-2-propenyl)- (9CI) (CA INDEX NAME)



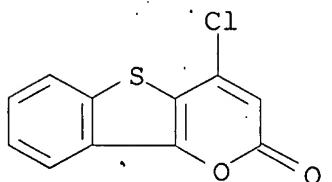
RN 6906-77-0 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy- (9CI) (CA INDEX NAME)



RN 56342-51-9 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-chloro- (9CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

AB 4-Hydroxypyranothianaphthene (I, R = OH, R1 = H) (II) reacted with PhNH2

in boiling HOCHMe2 to give the ring-cleavage product (III, R2 = COCH2CONHPh) whereas at higher temperature (e.g., in refluxing phenetole) IV (R3

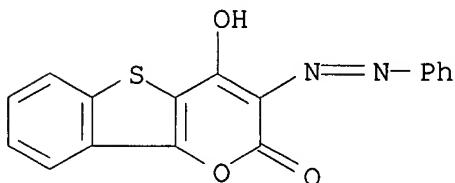
= Ph) was obtained; with H2NR4 (R4 = Bu, cyclopentyl, cyclohexyl, CH2CH2OH, CH2Ph) in boiling EtOH II gave only III [R2 = C(NHR4):CHCONHR4].

I (R = Cl, R1 = H) reacted with H2NR4 in EtOH to give the aminopyranothianaphthenes (I, R = NHR4, R1 = H), and I (R = OH, R1 = COCH:CHR5, R5 = Ph, C6H4OMe-p) reacted with H2NPh to give V.

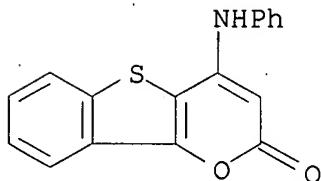
L4 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

10/552, 459

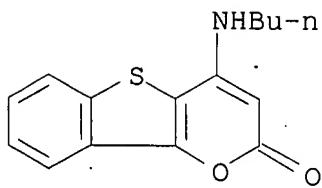
ACCESSION NUMBER: 1974:449595 CAPLUS
DOCUMENT NUMBER: 81:49595
TITLE: Action of amines on 4-hydroxy-2-oxo-2H-pyrano[3,2-b]thianaphthenes
AUTHOR(S): Ali, Mohamed I.; Samy, Salah M.
CORPORATE SOURCE: Fac. Sci., Univ. Cairo, Giza, Egypt
SOURCE: Egyptian Journal of Chemistry (1973), (Special), 169-77
CODEN: EGJCA3; ISSN: 0449-2285
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 2034-90-4P 2035-56-5P 53324-54-2P
53324-55-3P 53324-56-4P 53324-58-6P
53324-59-7P 53324-60-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2034-90-4 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(phenylazo)- (9CI)
(CA INDEX NAME)



RN 2035-56-5 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-(phenylamino)- (9CI) (CA INDEX NAME)

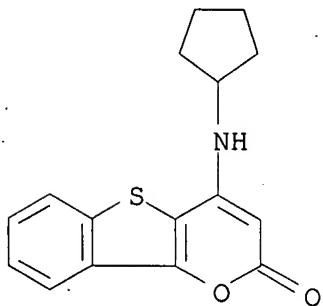


RN 53324-54-2 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-(butylamino)- (9CI) (CA INDEX NAME)



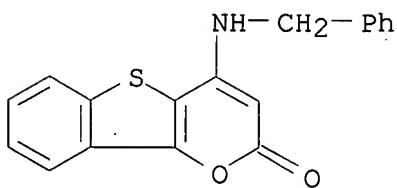
RN 53324-55-3 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-(cyclopentylamino)- (9CI) (CA INDEX NAME)



RN 53324-56-4 CAPLUS

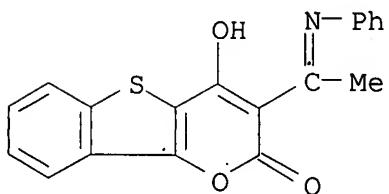
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-[(phenylmethyl)amino]- (9CI)
(CA INDEX NAME)



RN 53324-58-6 CAPLUS

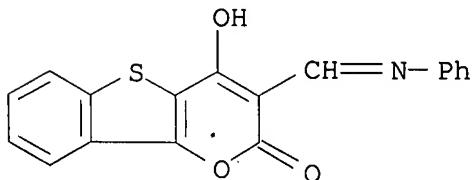
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one,
4-hydroxy-3-[1-(phenylimino)ethyl]-
(9CI) (CA INDEX NAME)

10/552, 459



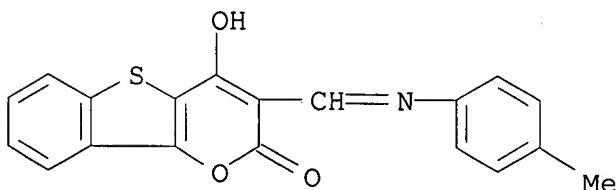
RN 53324-59-7 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-[(phenylimino)methyl]-
(9CI) (CA INDEX NAME)



RN 53324-60-0 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-[(4-methylphenyl)imino]methyl-
(9CI) (CA INDEX NAME)

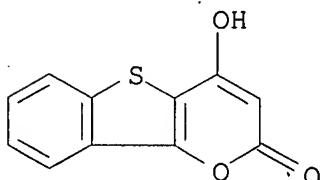


IT 6906-77-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with amines)

RN 6906-77-0 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy- (9CI) (CA INDEX NAME)



IT 2034-93-7 2035-18-9 2035-28-1

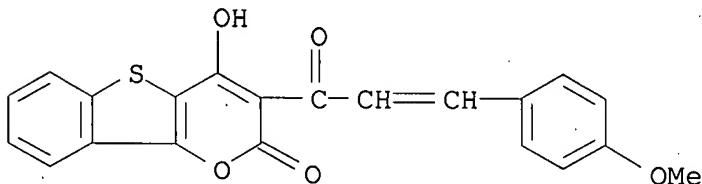
RL: RCT (Reactant); RACT (Reactant or reagent)

10/552, 459

(reaction of, with aniline)

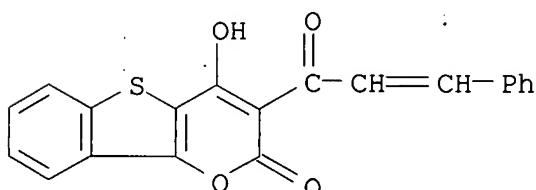
RN 2034-93-7 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one,
4-hydroxy-3-[3-(4-methoxyphenyl)-1-
oxo-2-propenyl]- (9CI) (CA INDEX NAME)



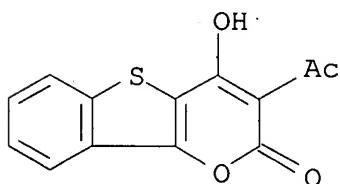
RN 2035-18-9 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(1-oxo-3-phenyl-2-
propenyl)- (9CI) (CA INDEX NAME)



RN 2035-28-1 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 3-acetyl-4-hydroxy- (9CI) (CA
INDEX
NAME)



GI For diagram(s), see printed CA Issue.

AB The pyranothianaphthene I ($R = OH$, $R_1 = H$) reacted with $PhNH_2$ at .apprx.80-140° with ring-opening to give II ($R_2 = COCH_2CONHPh$), whereas at .apprx.170° I ($R = NHPh$, $R_1 = H$) was obtained. Reaction in $HOAc$ at 118° yielded I ($R = NHPh$, $R_1 = H$), and II ($R_2 = Ac$) in addition to $PhNHAc$. Ring-opening also occurred in the reaction of I ($R = OH$, $R_1 = H$) with R_3NH_2 ($R_3 = Bu$, cyclopentyl, cyclohexyl, CH_2CH_2OH , CH_2Ph) or morpholine to give II [$R_2 = C(:CHCONHR_3)NHR_3$]. 3,3'-Methylenebis(4-

hydroxy-2-oxo-2H-pyrano[3,2-b]thianaph-thene) also reacted with PhNH₂ at 180° to give I. (R = NPh, R₁ = H), but remained unchanged when the reaction was carried out in refluxing EtOH. I (R = OH, R₁ = COCH:CHPh, COCH:CHC₆H₄OMe-p) both reacted with PhNH₂ to give I (R = OH, R₁ = CMe:NPh). Reaction of I (R = OH, R₁ = H) with HC(:NC₆H₄R₄-p)NHC₆H₄R₄-p (R₄ = H, Me) gave I (R = OH, R₁ = CH:NC₆H₄R₄-p).

L4 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1967:115525 CAPLUS

DOCUMENT NUMBER: 66:115525

TITLE: Thiophene derivatives. XVI. The Vilsmeier-Haack reaction with 3- and 4-methoxybenzo[b]thiophene

AUTHOR(S): Ricci, Adolfo; Balucani, Dante; Buu-Hoi, N. P.

CORPORATE SOURCE: Univ. Studi, Perugia, Italy

SOURCE: Journal of the Chemical Society [Section] C:

Organic

(1967), (8), 779-80

CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal

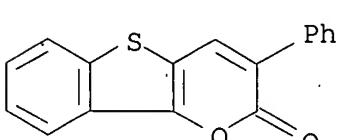
LANGUAGE: English

OTHER SOURCE(S): CASREACT 66:115525

IT 14854-19-4P, 2H-[1]Benzothieno[3,2-b]pyran-2-one, 3-phenyl-
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 14854-19-4 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 3-phenyl- (8CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

AB The Vilsmeier-Haack formylation of 3-methoxybenzo[b]thiophene (I) at moderate temperature leads to 2-formyl-3-methoxybenzo[b]thiophene, and under

more drastic conditions, to 3-chloro-2-formylbenzo[b]thiophene.

4-Methoxybenzo[b]thiophene undergoes formylation in the benzene ring, to give 7-formyl-4-methoxybenzo[b]thiophene.

L4 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:447553 CAPLUS

DOCUMENT NUMBER: 65:47553

ORIGINAL REFERENCE NO.: 65:8852e-h

TITLE: Syntheses of heterocycles. LXXXI. Substituted glyoxal

hydrazones

AUTHOR(S): Ziegler, E; Eichenseer, F

CORPORATE SOURCE:

SOURCE:

Univ. Graz, Austria

Monatshefte fuer Chemie (1966), 97(2), 391-7

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE:

Journal

LANGUAGE:

German

OTHER SOURCE(S):

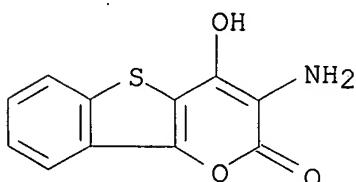
CASREACT 65:47553

IT 6906-80-5

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 6906-80-5 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, α -amino- β ,3-dihydroxy-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



IT 2034-90-4P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(phenylazo)-, δ -lactone 6906-77-0P,

Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy-, δ -lactone

6906-86-1P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy-

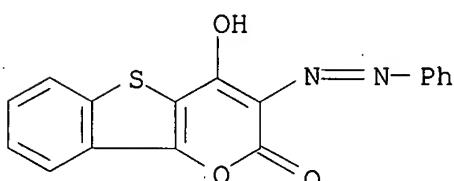
α -[(2-hydroxy-4-(methylsulfonyl)phenyl)azo]-, δ -lactone

RL: PREP (Preparation)

(preparation of)

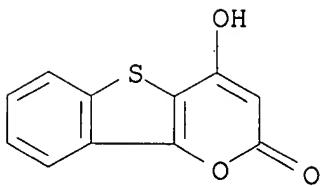
RN 2034-90-4 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(phenylazo)- (9CI)
(CA INDEX NAME)

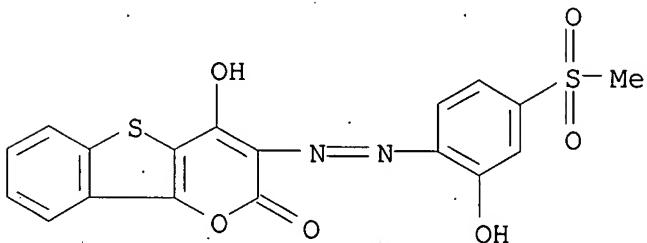


RN 6906-77-0 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy- (9CI) (CA INDEX NAME)



RN 6906-86-1 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β , γ -dihydroxy- α -[[2-hydroxy-4-(methylsulfonyl)phenyl]azo]-, δ -lactone (7CI, 8CI) (CA INDEX NAME)

AB cf. CA 65, 7137f. The syntheses were started with the known 4-hydroxy-2-oxoindeno[1,2-b]pyran (I), its O analogs (II), m. 212°, and its S analog (III), m. 257-9°, both of which were prepared by heating the 3benzyl derivative at 140° 10 min. with AlCl3

and

acidifying with HCl. I, II, and III were then coupled with diazotized aniline or 5-methylsulfonyl-2-aminophenol in about 10% Na2CO3 to give

IV,

m. 241°, V, m. 264°, VI, m. 253-5°, VII, m. 350°, VIII, m. 285°, and IX, m. 250°, in more than 80% yields. These upon hydrolysis with boiling 3% KOH in dilute EtOH

1-3

hrs. gave XI, m 188-90°, XII, m. 198-200°, XIII, m. 222° (diacetate m. 162°); XIV, m. 224-6°, and XV, m. 223°, in more than 75% yields. In the case of IV the intermediate carboxylic acid (X), m. 163°, was isolated in 75% yield by limiting the time of hydrolysis to 5 min. XI gave with CH2N2 a diacetate (XVa), m.

180°, and upon boiling with NH2OH in EtOH 48 hrs., the trioxime (XVI), m. 205-7°. With PhNHNH2·HCl and NaOAc it gave a pyrazolone (XVII), m. 223°. The N-methyl derivative, m. 205°, could be obtained either from XVa by the action of PhNHNH2 or from XVII with CH2N2.

L4 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

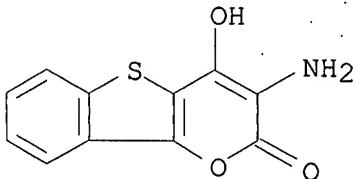
ACCESSION NUMBER: 1966:447552 CAPLUS

DOCUMENT NUMBER: 65:47552

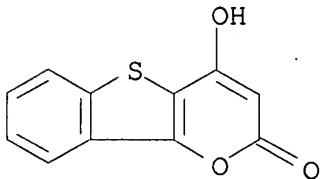
ORIGINAL REFERENCE NO.: 65:8852d-e

10/552, 459

TITLE: Removal of thiophene from benzene by freezing out
AUTHOR(S): Smol'yaninova, N. M.; Smol'yaninova, S. I.;
Potarskii,
V. K.
SOURCE: Izvestiya Tomskogo Politekhnicheskogo Instituta
(1965), 136, 93-6
From: Ref. Zh., Khim. 1966(5), Pt. II, Abstr. No.
5N116.
CODEN: ITPKAM; ISSN: 0368-0487
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT 6906-80-5
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 6906-80-5 CAPLUS
CN Benzo[b]thiophene-2-acrylic acid, α -amino- β ,3-dihydroxy-,
 δ -lactone (7CI, 8CI) (CA INDEX NAME)



IT 6906-77-0P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy-,
 δ -lactone
RL: PREP (Preparation)
(preparation of)
RN 6906-77-0 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy- (9CI) (CA INDEX NAME)



AB The dependence of C6H6 yield, its thiophene content, and the degree of purification on the number of crystallization steps from a mixture of xylenes or MeOH was studied. Thiophene can be removed from C6H6 by a freezingout method with MeOH as solvent. A high-purity product can be obtained by multiple purifications with a high recirculation factor.

L4 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1965:90854 CAPLUS
DOCUMENT NUMBER: 62:90854
ORIGINAL REFERENCE NO.: 62:16218g-h,16219a-h,16220a-c
TITLE: Synthesis of substituted linear furano[2,3-g][1]benzopyrones and [3,2-b]thianaphthenopyrones
AUTHOR(S): Mustafa, A.; Asker, W.; Hishmat, O. H.; Ali, M. I.; Mansour, A. K. E.; Abed, N. M.; Khalil, K. M. A.; Samy, S. M.
CORPORATE SOURCE: Cairo Univ.
SOURCE: Tetrahedron (1965), 21(4), 849-59
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 62:90854
IT 2034-88-0P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(p-tolylazo)-, δ -lactone 2034-89-1P,
Benzo[b]thiophene-2-acrylic acid, α -[(p-chlorophenyl)azo]- β ,3-dihydroxy-, δ -lactone 2034-90-4P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(phenylazo)-, δ -lactone 2034-91-5P, Benzo[b]thiophene-2-acrylic acid, α -acetamido- β ,3-dihydroxy-, δ -lactone 2034-92-6P,
Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -nitro-, δ -lactone 2034-93-7P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(p-methoxycinnamoyl)-, δ -lactone 2035-18-9P, Benzo[b]thiophene-2-acrylic acid, α -cinnamoyl- β ,3-dihydroxy-, δ -lactone 2035-19-0P,
Benzo[b]thiophene-2-acrylic acid, α -acetyl- β ,3-dihydroxy-, δ -lactone, methylphenylhydrazone 2035-20-3P,
Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(N-phenylbutyrimidoyl)-, δ -lactone 2035-21-4P,
Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(N-phenylpropionimidoyl)-, δ -lactone 2035-22-5P,
Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(N-p-tolylacetimidoyl)-, δ -lactone 2035-23-6P,
Benzo[b]thiophene-2-acrylic acid, α -(N-butylacetimidoyl)- β ,3-dihydroxy-, δ -lactone 2035-24-7P, Benzo[b]thiophene-2-acrylic acid, α -(N-ethylacetimidoyl)- β ,3-dihydroxy-, δ -lactone 2035-25-8P, Benzo[b]thiophene-2-acrylic acid, α -acetimidoyl- β ,3-dihydroxy-, δ -lactone 2035-26-9P, Benzo[b]thiophene-2-acrylic acid, α -butyryl- β ,3-dihydroxy-, δ -lactone 2035-27-0P,
Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -propionyl-, δ -lactone 2035-28-1P, Benzo[b]thiophene-2-acrylic acid, α -acetyl- β ,3-dihydroxy-, δ -lactone 2035-29-2P,
Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy-, δ -lactone, benzoate 2035-30-5P, Benzo[b]thiophene-2-acrylic acid, 3-hydroxy- β -p-toluidino-, δ -lactone 2035-56-5P,
Benzo[b]thiophene-2-acrylic acid, β -anilino-3-hydroxy-, δ -lactone 2239-09-0P, Benzo[b]thiophene-2-acrylic acid, α -(N-sec-butylacetimidoyl)- β ,3-dihydroxy-, δ -lactone 2239-10-3P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(phenylacetyl)-, δ -lactone 2239-11-4P,

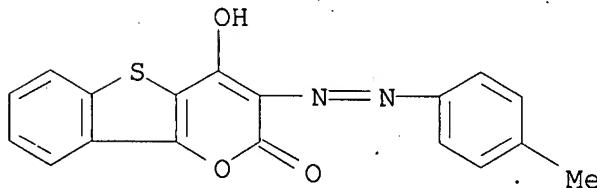
10/552, 459

Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -isobutyryl-, δ -lactone 2864-01-9P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(N-isobutylacetimidoyl)-, δ -lactone

RL: PREP (Preparation)
(preparation of)

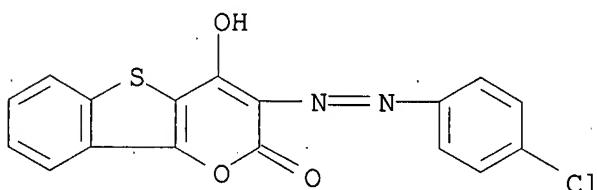
RN 2034-88-0 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(p-tolylazo)-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



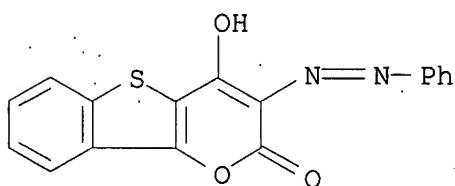
RN 2034-89-1 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 3-[(4-chlorophenyl)azo]-4-hydroxy- (9CI) (CA INDEX NAME)



RN 2034-90-4 CAPLUS

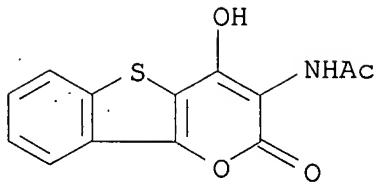
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(phenylazo)- (9CI)
(CA INDEX NAME)



RN 2034-91-5 CAPLUS

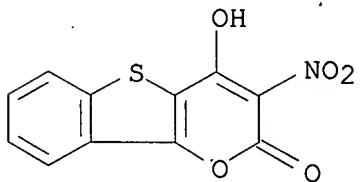
CN Benzo[b]thiophene-2-acrylic acid, α -acetamido- β ,3-dihydroxy-, δ -lactone (7CI, 8CI) (CA INDEX NAME)

10/552, 459



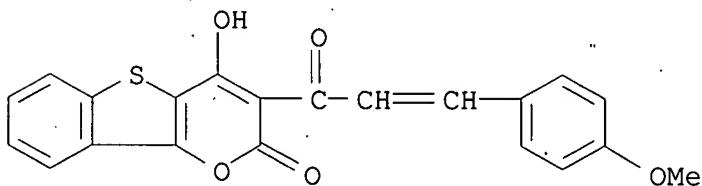
RN 2034-92-6 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -nitro-,
 δ -lactone (7CI, 8CI) (CA INDEX NAME)



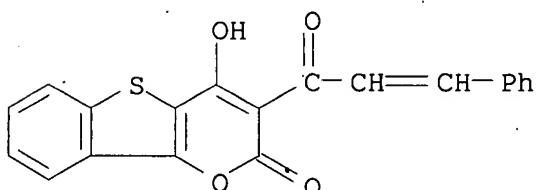
RN 2034-93-7 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one,
4-hydroxy-3-[3-(4-methoxyphenyl)-1-
oxo-2-propenyl]- (9CI) (CA INDEX NAME)



RN 2035-18-9 CAPLUS

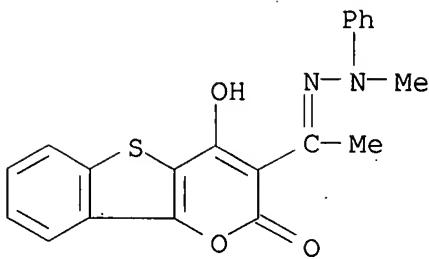
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(1-oxo-3-phenyl-2-
propenyl)- (9CI) (CA INDEX NAME)



RN 2035-19-0 CAPLUS

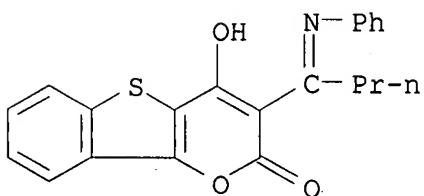
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-[1-
(methylphenylhydrazone)ethyl]- (9CI) (CA INDEX NAME)

10/552,459



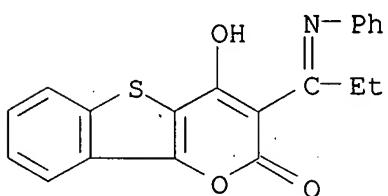
RN 2035-20-3 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β , δ -dihydroxy- α -(N-phenylbutyrimidoyl)-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



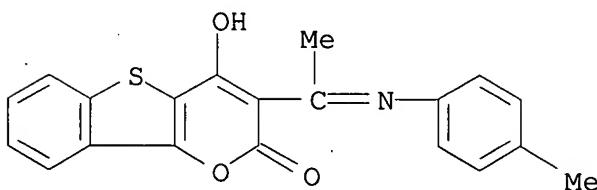
RN 2035-21-4 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β , δ -dihydroxy- α -(N-phenylpropionimidoyl)-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



RN 2035-22-5 CAPLUS

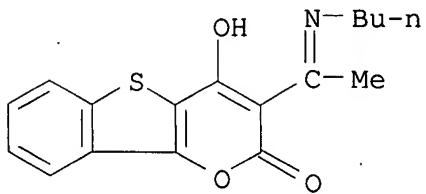
CN Benzo[b]thiophene-2-acrylic acid, β , δ -dihydroxy- α -(N-p-tolylacetimidoyl)-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



RN 2035-23-6 CAPLUS

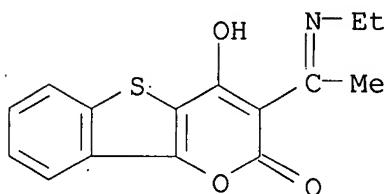
10/552, 459

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 3-[1-(butylimino)ethyl]-4-hydroxy-
(9CI) (CA INDEX NAME)



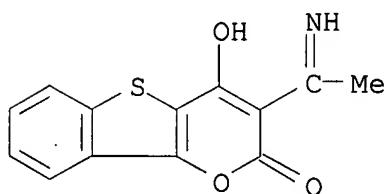
RN 2035-24-7 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, α -(N-ethylacetimidoyl)- β ,3-dihydroxy-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



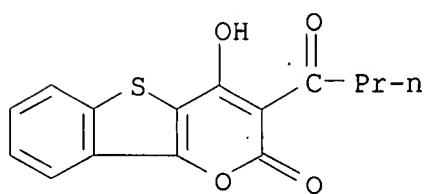
RN 2035-25-8 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, α -acetimidoyl- β ,3-dihydroxy-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



RN 2035-26-9 CAPLUS

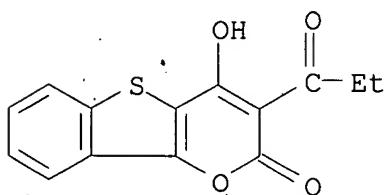
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(1-oxobutyl)- (9CI)
(CA INDEX NAME)



10/552,459

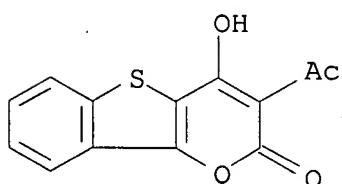
RN 2035-27-0 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -propionyl-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



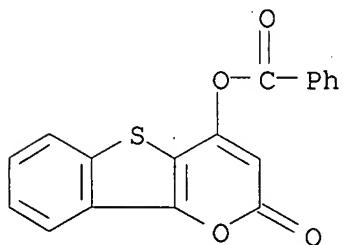
RN 2035-28-1 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 3-acetyl-4-hydroxy- (9CI) (CA INDEX NAME)



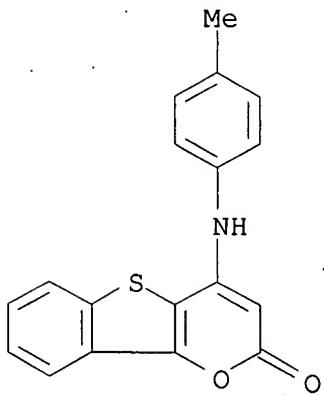
RN 2035-29-2 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy-, δ -lactone, benzoate (7CI, 8CI) (CA INDEX NAME)



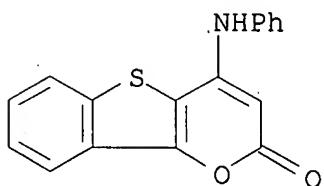
RN 2035-30-5 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, 3-hydroxy- β -p-toluidino-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



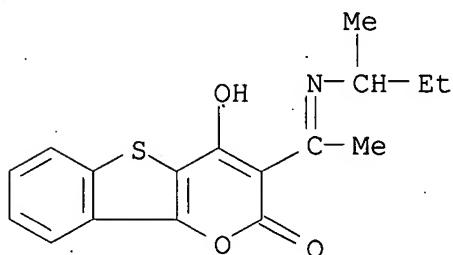
RN 2035-56-5 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-(phenylamino)- (9CI) (CA INDEX NAME)



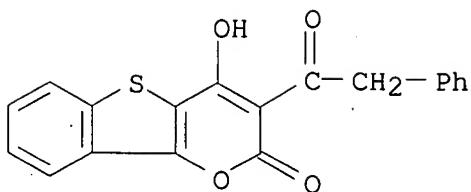
RN 2239-09-0 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, α -(N-sec-butylacetimidoyl)- β ,3-dihydroxy-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



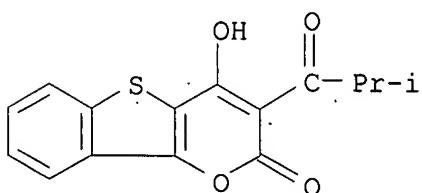
RN 2239-10-3 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(phenylacetyl)-, δ -lactone (8CI) (CA INDEX NAME)



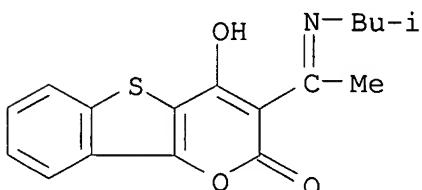
RN 2239-11-4 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β , δ -dihydroxy- α -isobutyryl-, δ -lactone (7CI, 8CI). (CA INDEX NAME)



RN 2864-01-9 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-[1-(2-methylpropyl)imino]ethyl- (9CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

AB Dry PhNO₂ (10 ml.) and 0.6 g. acetoxy-2,3-diphenylbenzofuran (I, R = Ac,

R1 = H) kept 5 days at 25° with 1 g. anhydrous AlCl₃ and the dried product extracted with ligroine (b. 100-40°) gave 73% I (R = H, R1 = Ac) (II), m. 157° (alc.). I (R = R1 = H) (III) (2.8 g.) and 3.5 g. AlCl₃ in 25 ml. PhNO₂ kept 5 days at 25° with 8 ml. AcCl, extracted with ligroine and the crystalline product recrystd. from C₆H₆ yielded 12%

4-acetyl-5-hydroxy-2,3-diphenylbenzofuran, m. 291°. Concentration of the ligroine mother liquor gave 65% II. III (2.8 g.), and 1.86 g.

PhCH:CHCOCl

refluxed 3 hrs. with 3.4 g. AlCl₃ in 25 ml. CS₂ and the product extracted with

petr. ether (b. 40-60°) yielded 95% I (R = PhCH:CHCO, R1 = H), m. 132° (alc.), converted by keeping in PhNO₂ with AlCl₃ to I (R = H,

R₁ = PhCH:CHCO), m. 184°, giving a reddish brown color with aqueous FeCl₃. Treatment of III with PhCH:CHCOCl under Friedel-Crafts conditions

gave 85% yield. II (1 g.) in 20 ml. EtOAc refluxed 1 hr. with 1 g. finally divided Na and the mixture decomposed with ice-H₂O, washed with Et₂O

and the aqueous layer acidified with dilute HCl yielded 82% I (R = H,

R₁ = AcCH₂CO) (IV). II (1 g.) and 4 ml. Et₂CO₃ shaken 5 min. with 0.5 g. Na at

25° and the mixture kept at 100° 4 hrs., the product taken up in H₂O and the solution washed with Et₂O, the aqueous layer acidified with cold

dilute HCl gave 0.7 g.

2,3-diphenyl-8-hydroxy-6H-furano[2,3-g][1]benzopyran-

6-one (V), m. 288-90° (decomposition), N.M.R. singlets at 7.92, 7.18 ppm. and a signal group at 7.4 ppm. IV (1 g.) refluxed 1 hr. in 30 ml. 25% aqueous H₂SO₄ and the solution neutralized with Na₂CO₃ yielded 77% 2,3-diphenyl-6-methyl-8H-furano[2,3-g][1]benzopyran-8-one (VI), m. 211-12°, N.M.R. signals at 8.24, 7.4, 6.14, 2.35 ppm. The substitution of the 2- and 3-Ph groups effected the stabilization of V

and

VI against the action of mineral acids. III refluxed with H₂C:CHCH₂Br and

K₂CO₃ in dry Me₂CO 12 hrs. yielded 55% I (R = CH₂:CHCH₂, R₁ = H), m. 72°, rearranged by refluxing 3 hrs. in PhNMe₂ and acidifying the product to give I (R = H, R₁ = CH₂:CHCH₂), m. 83°, giving a red color with concentrated H₂SO₄. The thianaphthene (VII, R = H, R₁ =

OH) (VIII)

(1 g.) (Smiles and Hart, CA 18, 390) heated with 1 ml. PhNH₂ in 20 ml. alc. or in the absence of alc. 4 hrs. on a water bath yielded 85% α-(3-hydroxy-2-thianaphthenoyl)acetanilide (IX, R = Ph) (X), m. 188-90° (alc.). Similarly VIII and p-MeC₆H₄NH₂ heated in alc. gave 60% IX (R = p-MeC₆H₄), m. 199° (alc.). X (0.6 g.) and 1 ml. PhNH₂ heated 1.5 hrs. at 180° and the product triturated with cold alc. gave VII (R = H, R₁ = NHPh) (XI), m. 280°. Concentration of the mother liquor gave a compound tentatively formulated as IX [R = C(NHPh):CHCONHPh],

m. 222°, giving a green color with aqueous FeCl₃. VIII heated 1.5 hrs. with p-MeC₆H₄NH₂ gave 71% VII (R = H, R₁ = p-MeC₆H₄NH), m. 269-70° (alc.). VIII benzoylated and crystallized from alc. yielded 75% VII (R = H, R₁ = OBz), m. 162°, converted by refluxing with PhNH₂ in alc. to X.

VII (R = H, R₁ = Cl) refluxed in alc. with PhNH₂ yielded XI. VIII (0.01 mole), 8 ml. RCO₂H, and 10 ml. POC₁₃ refluxed 45 min. and the mixture

poured

onto ice, the precipitate washed with cold H₂O and dried gave the acyl derivs.

VII [R, R₁, m.p. (solvent), and % yield given]: Ac, OH (XII), 189-90° (AcOH), 76; EtCO, OH (XIII), 180-1° (AcOH), 65; PrCO, OH (XIV), 170-1° (AcOH), 76; Me₂CHCO, OH, 172-3°

(AcOH), 70; PhCH₂CO, OH, 205° (dioxane), 71. The acyl derivs.

XII-XIV (0.5 g.) refluxed 3-4 hrs. with excess of the appropriate amine (8

hrs. with NH₄OAc) in 30 ml. alc. gave the corresponding amino or imino derivs. (XV) as listed [R, R₁, m.p. (solvent), and % yield given]: Me,

H,
288-90° (xylene), 80: Me, Et, 224° (alc.), 73; Me, Bu,
128-9° (aqueous alc.), 90; Me, EtMeCH, 139-40° (aqueous alc.), 83;
Me, Me₂CHCH₂, 109-10° (aqueous alc.), 90; Me, p-MeC₆H₄, 228-30°
(AcOH) 82; Et, Ph, 200° (alc.), 80; Pr, Ph, 145° (alc.), 72.
XII and MePhNNH₂ refluxed in alc. 3 hrs. and the product recrystd.

yielded

82% XV (R = Me, R₁ = NMePh), m. 168°. XII heated with BzH in the presence of a drop of piperidine 1 hr. on a water bath yielded 65% VII (R

= COCH:CHR₂, R₁ = OH) (XVI, R₂ = Ph), m. 230° (dioxane-H₂O).

Similarly was obtained 60% XVI (R₂ = p-MeOC₆H₄), m. 220° (dioxane).

The ir spectrum of XII showed a broad OH absorption band as well as a strong peak in good agreement with the spectra of α,β -unsatd. δ -lactones. VIII gave bands at 7.55 and 5.87 μ but displayed no free OH peak, indicating a strongly H-bonded OH group. VIII kept 16 hrs.

at 25° in AcOH with concentrated HNO₃ gave VII (R = NO₂, R₁ = OH), m. 215° (AcOH), reduced with Zn dust in 1:1 AcOH-Ac₂O to give VII (R = NHAc, R₁ = OH), m. 250-2°. VIII (1 g.) in 100 ml. alc. containing 2.5 g. NaOAc.3H₂O treated with 0.005 mole of the appropriate aryl diazonium chloride gave 94% VII (R = PhN:N, R₁ = OH), m. 260°, converted by reductive acetylation to yield 70% VII (R = NHAc, R₁ = OH), m. 250-2°; 84% VII (R = p-MeC₆H₄N:N, R₁ = OH), m. 250° (AcOH); and 85% VII (R = p-ClC₆H₄N:N, R₁ = OH), m. 257° (AcOH). EtOH (10 ml.) containing 0.001 mole 2-acetyl-3-hydroxythianaphthene, treated

with

0.0015 mole of the appropriate aldehyde, RCHO, and the mixture refluxed 30

min. with 4 ml. 10% alc. NaOH, kept at 25°, and acidified with dilute HCl, filtered and the dried products crystallized from AcOH gave the 2-cinnamoyl-3-hydroxythianaphthenes (XVII) (R, m.p., and % yield): Ph, 154°, 50; p-MeOC₆H₄ (XVIII), 175°, 60; p-MeC₆H₄ (XIX), 130°, 65; 3,4-(OCH₂O)C₆H₃ (XX), 199°, 75; 3,4-(EtO)C₆H₃ (XXI), 150°, 50; p-ClC₆H₄ (XXII), 166°, 70. Each of the chalcones XX-XXII (0.5 g.) refluxed 10-15 hrs. with 0.5 g. SeO₂ in 8 ml.

isoamyl alc. and the filtered solution evaporated, the residue washed with cold

alc. and crystallized from alc. gave the 2-aryl-4-oxo-4H-pyrano[3,2-b]thianaphthenes (XXIII) (R, m.p., and % yield given): 3,4-(OCH₂O)C₆H₃, 266-7°, 80; 3,4-(EtO)C₆H₃, 170-1°, 65; p-ClC₆H₄, 235°, 80. Each of the chalcones XVIII-XXI (0.5 g.) and 0.5 g. of the appropriate thiol heated 4 hrs. on a water bath with 1-2 drops of piperidine, the product triturated with petr. ether and the solid crystallized

gave the thiol adducts (XXIV) [R, R₁, m.p. (solvent) and % yield given]:

p-MeOC₆H₄, p-MeC₆H₄ (XXV), 101-2° (alc.), 60; p-MeC₆H₄, Ph (XXVI), 110-12° (AcOH), 55; p-MeC₆H₄, m-MeC₆H₄, 92-3° (alc.), 60; p-MeC₆H₄, p-MeC₆H₄, 105-6° (alc.), 60; 3,4-(OC-H₂O)C₆H₃, Ph, 125-6° (AcOH), 58; 3,4-(OCH₂O)C₆H₃, o-MeC₆H₄, 132-3° (AcOH), 60; 3,4-(OCH₂O)C₆H₃, m-MeC₆H₄, 106° (AcOH), 60; 3,4-(OCH₂O)C₆H₃, p-MeC₆H₄, 135-6° (AcOH), 60; 3,4-(EtO)C₆H₃, p-MeC₆H₄, 105° (alc.), 50. XXVI (0.5 g.) in 10 ml. alc. refluxed 30 min. with 3 ml.

5%

alc. KOH and the product taken up in 10 ml. cold alc., acidified with cold dilute HCl and the product crystallized from AcOH gave XIX. Treatment of XVIII

or XX in AcOH with 30% H₂O₂ gave the dioxides [XXVII, R = p-MeOC₆H₄, 3,4-(OCH₂O)C₆H₃] (XXVIII, XXIX), m. 215° (AcOH), 271-3° (PHCl), in 61 and 70% yields, resp. XXIX was also obtained in 52% yield

by treatment of the thiol adduct XXIV [R = 3,4-(OCH₂O)C₆H₃, R₁ = p-MeC₆H₄]

with H₂O₂ in AcOH. XXVIII and XXIX formed unstable thiol adducts with p-thiocresol.

L4 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

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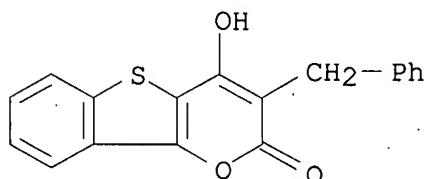
IT 108237-18-9P, Benzo[b]thiophene-2-acrylic acid, α-benzyl-β,3-dihydroxy-, δ-lactone

RL: PREP (Preparation)

(preparation of)

RN 108237-18-9 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, α-benzyl-β,3-dihydroxy-, δ-lactone (6CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

AB cf. CA 53, 20044g. The reactions of a number of cyclic ketones with PhCH₂CH(CO₂C₆H₃Cl₂-2,4)₂ (I) were reported. 1-Menthone (2 g.) and 4.84 g.

I heated 90 min. at 270°, the crude product steam distilled, the residual material dissolved in NaOH and repptd. with HCl, the material (2.8 g.) rubbed with 4:1 cyclohexane-C₆H₆, allowed to stand several days,

and recrystd. from C₆H₆ or EtOAc gave 3-benzyl-4-hydroxy-5-methyl-8-isopropyl-5,6,7,8-tetrahydrocoumarin, m. 170°.

1-Phenyl-3-methyl-5-pyrazolone (3.5 g.) and 4.8 g. I heated 20 min. at 190° and the product rubbed with C₆H₆ and then EtOH gave 2.2 g.

1-phenyl-3-methyl-4-hydroxy-5-benzyl-6-oxo-1,6-dihydropyrano[2,3]pyrazole, m. 226-7° [dioxane or (Cl₂CH)₂]. Benzo-suberone (2.5 g.) and 9 g. I heated 1 hr. at 260-70° and the crude product rubbed with petr. ether gave 4.4 g. 3-benzyl-4-hydroxy-2-oxobenzo[a]pyran [2,3-b]cycloheptadiene (II), m. 231° (EtOAc, EtOH, dioxane, or PhCl). II (1.6 g.) and 3.2 g. AlCl₃ heated 10 min. at 140°, the mixture decomposed at 0° with dilute HCl, and the crude product repptd. from NaOH with HCl gave 1.1 g. corresponding debenzylated product, m. 196-7° (PhCl or xylene): α-Tetralone (1.5 g.) and 2.4 g. I heated 30 min. at 255° and the crude product rubbed with C₆H₆ gave 0.95 g. 3-benzyl-4-hydroxy-5,6-dihydro-7,8-benzocoumarin (III), m. 222-3° (PhCl or AcOH). III (0.43 g.) and 0.7 g. AlCl₃ heated at 150° and the mixture decomposed with dilute HCl gave 0.2 g. 4-hydroxy-7,8-benzocoumarin, m. 276° (dilute EtOH, PhCl, or AmOAc). 1,4-Cyclohexanedione (0.2 g.) and 2.4 g. I heated 20 min. at 260°, cooled, rubbed with C₆H₆, and recrystd. from PhCH₂OH, PhNO₂, or p-cresol.

gave 0.4 g.

4,8-dihydroxy-3,7-dibenzyl-2,6-dioxo-1,5-dioxa-1,2,5,6,9,10-hexahydroanthracene, m. 365° (decomposition); diacetate m. 256-7° (xylene or PhCl). Coumaranone (0.6 g.) and 2.4 g. I heated 10 min. at 255° and the product rubbed with C₆H₆ gave 0.9 g. 3-benzyl-4-hydroxy-2-oxopyrano[3,2-b]benzofuran, m. 245-7° (PhNO₂, AcOH, or Tetralin). 3-Hydroxythianaphthene and 2.9 g. I heated 10 min. at

255° and the product rubbed with C₆H₆ gave 1.3 g.

3-benzyl-4-hydroxy-2-oxopyrano[3,2-b]thianaphthene, m. 247° (EtOH, AcOH, or PhNO₂). 1-Hydrindone (0.65 g.) and 2.4 g. I heated 45 min. at 250° and the product (0.9 g.) rubbed with C₆H₆ gave 3-benzyl-4-hydroxy-2-oxoindeno[1,2-b]pyran (IV), m. 273° (PhNO₂). IV (0.96 g.) and 1.35 g. AlCl₃ heated 7 min. at 140-50°, the product repptd. from aqueous NaOH with HCl, and crystallized from dioxane-H₂O with

C gave 0.4 g. 4-hydroxy-2-oxoindeno[1,2-b]pyran, m. 244-5° (decomposition). Flavanone (1.12 g.) and 2.9 g. I heated 1 hr. at 270-80°, allowed to stand 1 day, and rubbed with 1:1 C₆H₆-cyclohexane gave 0.5 g.

1-hydroxy-2-benzyl-3-oxo-10-phenyl-4,9-dioxa-3,4,9,10-tetrahydrophenanthrene, m. 218° (EtOH, PhCl, or AcOH);

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monoacetate m. 204.5° (AcOH). peri-Naphthindandione (0.36 g.) and 1.2 g. I heated 35 min. at 250° gave 0.6 g. 8-hydroxy-9-benzyl-7,10-dioxo-11-oxa-10,11-dihydrobenzanthrene, m. 256-7° [dioxane, (Cl₂CH)₂, or PhNO₂]. BzCH₂ (1.12 g.) and 2.9 g. I heated 1 hr. at 270°, the 2,4-C₁₂C₆H₃OH distilled, and the product rubbed with 1:1 C₆H₆-cyclohexane gave 0.4 g. 3-benzyl-4-hydroxy-6-phenyl-2-pyrone, m. 251° (EtOH or AcOH). Acetylacetone monoanil (1.8 g.) and 4.8 g. I heated 12 min. at 260° gave 1.9 g. O.CO.C(CH₂Ph):C(OH).C(CMe:NPh):C Me, m. 247-8° [(Cl₂CH)₂-EtOH or PhNO₂].

=> log y

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| FULL ESTIMATED COST | 85.26 | 257.57 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -12.48 | -12.48 |

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